Sustainable Process Engineering
Micro Flow Chemistry & Synthetic Methodology

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

Predicting reaction performance in sulfonamide electrochemical synthesis using machine learning

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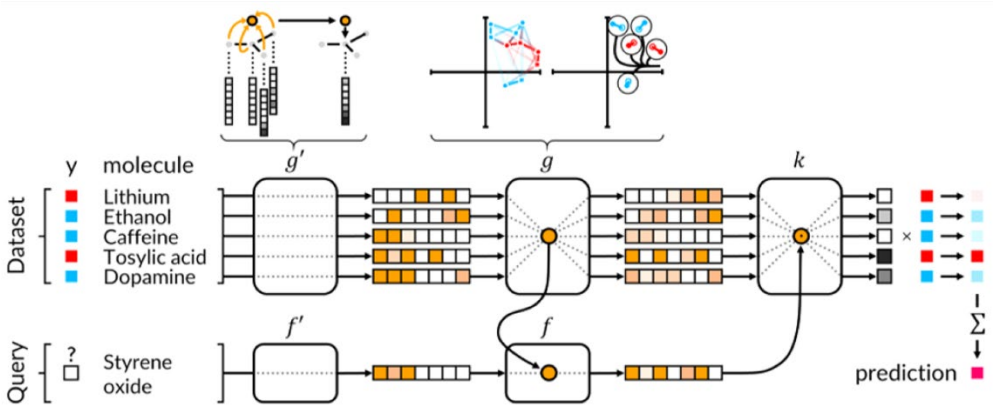
Introduction

Machine learning methods are becoming integral to scientific inquiry in numerous disciplines. It was demonstrated that machine learning can be used to predict the performance of a synthetic reaction in multidimensional chemical space using data obtained via experimentation.

Project summary

Using molecular descriptors as inputs and reaction yield as outputs, a random forest algorithm provides significantly improved predictive performance over linear regression analysis. The random forest model will also be applied to sparse training sets and out-of-sample prediction, suggesting its value in facilitating adoption of synthetic methodology.



Project goals

Optimize model pipeline using Python and ChemSAR platform

Contact information

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